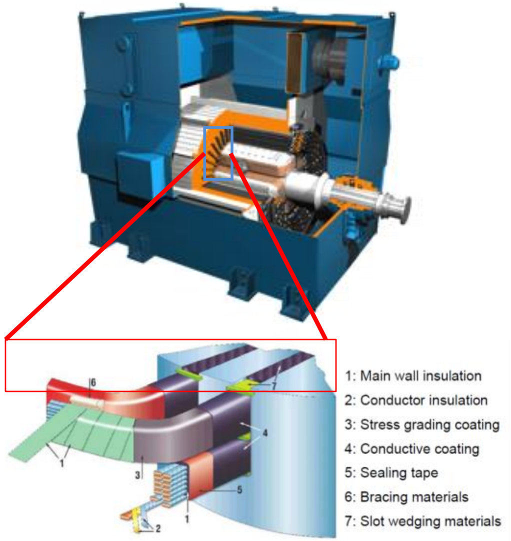
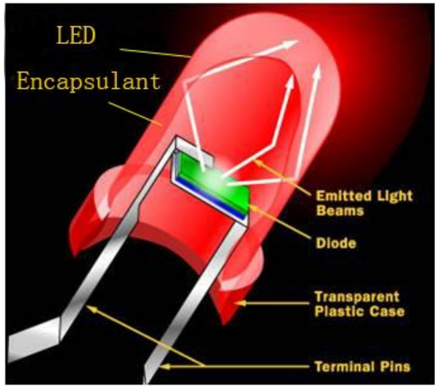
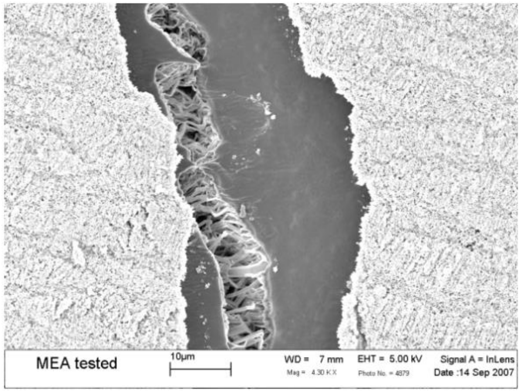
Breakout Report on Polymer Composites

Identification of Grand Challenges







Breakout Polymer Composites

- Chairs:
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Committee: Members	
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Greg Schoeppner	AFRL
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Polymer Composites

- Polymer composites consist of polymers containing micro and/or nano constituents to produce enhanced multifunctional properties.
- Properties derive from composition and micro/nano structure (constituents, interface and polymer)
- Two primary classes of polymer composites:
  – Light weight structural materials
  – Multifunctional polymer materials with enhanced optical, thermal, electric/dielectric and ionic performance.

What is the answer?

- Paradigm shift in simulation comprehensiveness: design for manufacturing and performance
  - replace the building block approach with simulation and **test for validation**
  - certify products in a manner that allows for composition and processing to be adjustable **without recertification**
- Combine experiments **curated data, data mining and validated simulation** for *a priori* materials design
- Build the **simulation base in design and manufacturing**
- Understand the **origins of uncertainty** and control them
- Simulation tools can guide understanding of **propagation of uncertainty in design and manufacturing**
- Make interconnected **simulation tools broadly available** for designers, materials suppliers and manufacturers

Polymer Composites MGI

PURDUE ENGINEERING

Materials/product engineers need to be able to _______	**Which materials scientists could enable by _______**
Develop and validate composite simulation models. A serious UQ effort to quantify "model form error" in our simulations.	Full 3-D imaging of 1000 cm^3 cube real or full scale composites with resolution at level of constituents, orientation, distribution etc.
Simulate composite manufacturing processes to predict microstructure and variability	Developing measurements and models to determine non-equilibrium , polymer molecular mass, and chemical functionality changes during cure in a 3-D part
Validate simulation tools for composite performance	Developing an open curated database of composite test and simulation data

Polymer Composite Needs

If materials scientists could ________, then new pathways of materials discovery would be possible.

- Connecting multi-scale simulation that integrates molecular modeling into existing micro and macro scale simulations
- Need models to predict onset and propagation of damage
- Need multi-physics/chemistry kinetic models of all processing relevant phenomena
- Need models for adhesion of multi-material systems to integrate interaction of polymer, constituent and interphase properties
- Create curated and discoverable data bases sufficient for discovery of optimum systems
- Create simulation libraries of previous studies with intelligence
- Rapidly measure properties at all scales

Polymer Composites Development

- Reduction in the huge cost of polymer composites **development** is still needed.
- Primary costs are associated with engineering required for product certification (especially for aircraft) via experiment dominated “building-block-approach”.
- Material supplier OEM interaction **process too slow and costly**
- Cost reduction via replacement of a portion of experiments by **validated simulations using the MGI approach consisting of physically realistic multi-scale models**, starting at the atomistic level and extending continuously to the macroscopic scale to enable accurate prediction of full scale performance.
- A **simulation suite with individual tools ranked by a technology readiness level system** for measured validation and verification (tool maturity level).

Polymer Composites Discovery

- Composite performance is limited by current materials, both polymer and reinforcement, therefore material **discovery** is required.
- Taking the MGI approach in the composites will produce the largest impact if efforts are focused on discovery of:
  - new polymer and constituent combinations to produce enhanced performance
  - conventional composites with multifunctional performance ((electrical conductivity)
  - tailorable polymer chemistries to enable enhanced processing
  - materials with improved life-cycle performance
  - recyclable and sustainable systems and methods
  - methods for control of nanoparticle-network meso-structure.

Molecular Modeling Advances

Describe microstructure more realistically. We often assume very regular materials, with perfect stoichiometry down to the few nanometers, no significant defects, gradients in composition, etc. This is particularly important near the fibers.

Perform “reactive MD simulations” where chemical bonds are allowed to break and form as needed to predict ultimate properties. Reactive interatomic potentials (like ReaxFF) exist for this but have not been used in the field.

Defect propagation will require very large-scale Simulations.

A serious UQ effort to quantify “model form error” in our simulations. This would require very
detailed experiments where the molecular structure is well known in samples small enough
to simulated directly.

Relaxation time scales of long-chain polymers is well over MD timescales and this continues
to be a problem

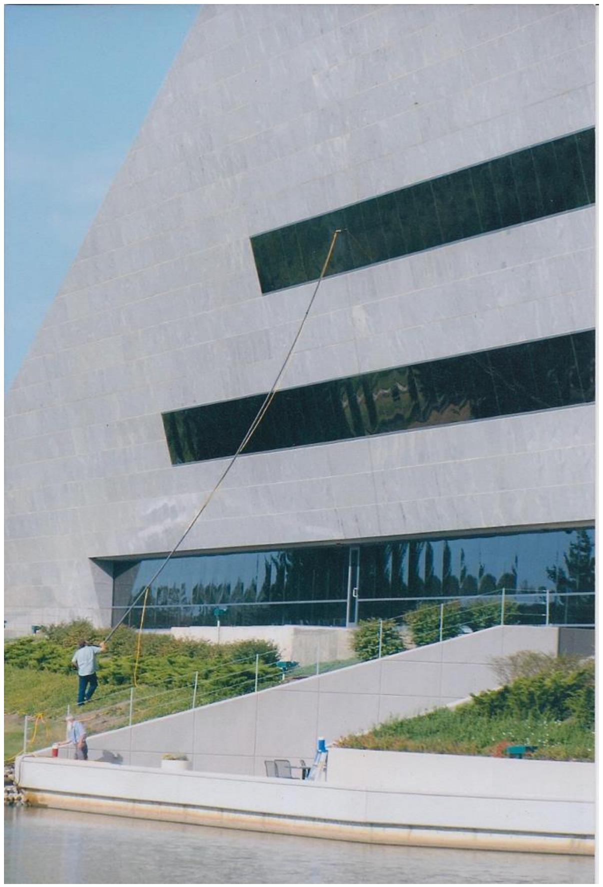
Military Aircraft and Composites since 1971







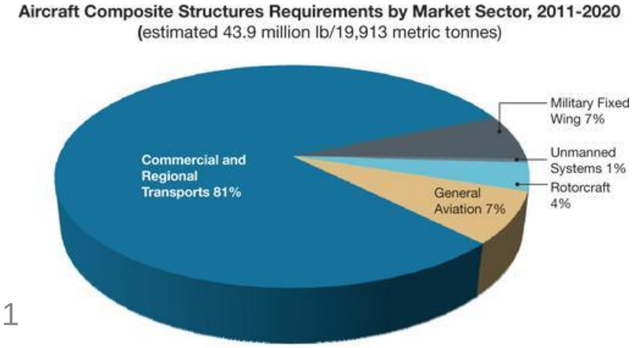
Carbon fiber composites have entered the mainstream



Commercial aviation

Airbus 350

Engine blades and shroud

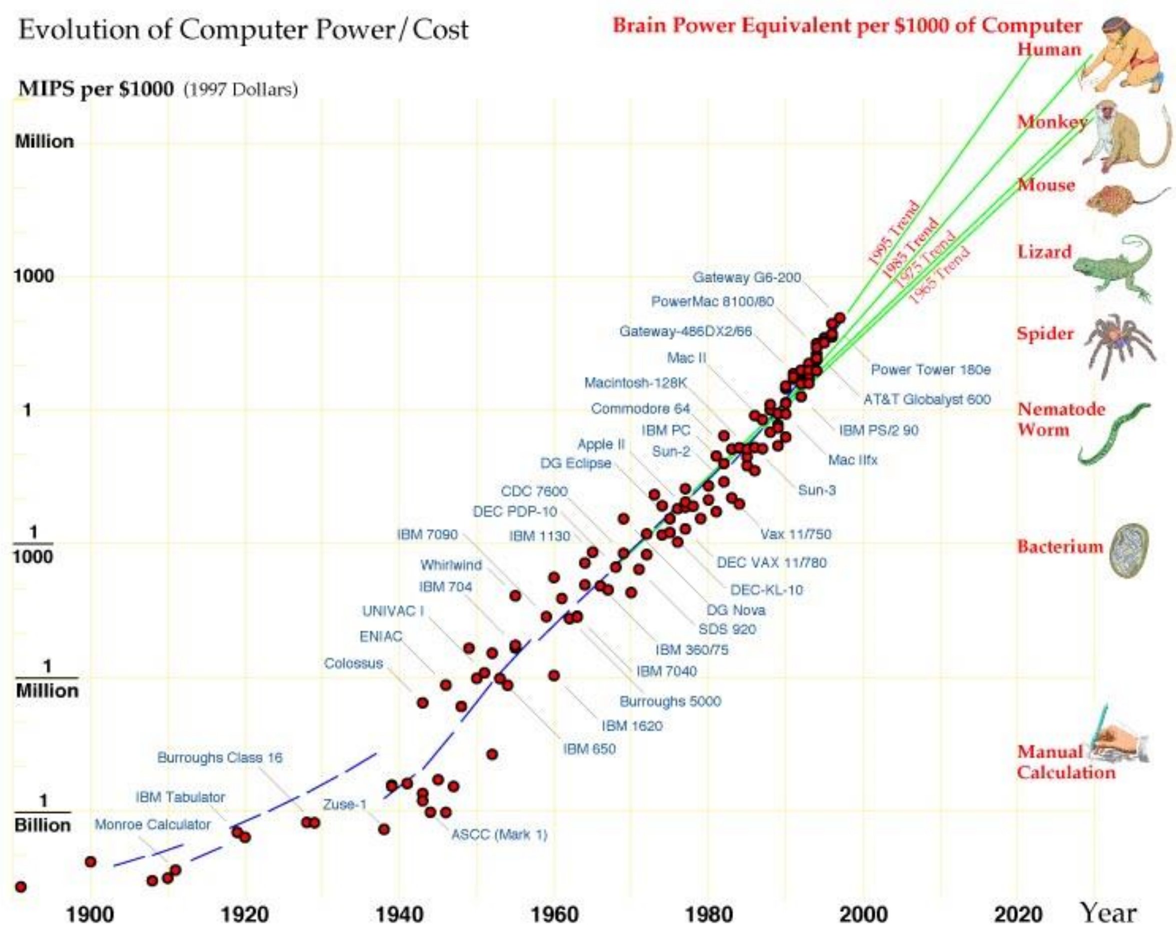


Boeing 787

After 50 years of progress in composites research

- Commercial aircraft are a reality
- Defense aerospace composites are pervasive
- The world-wide failure analysis proved that prediction of strength has been elusive
- Yet we design successfully
- But, we do so with significantly conservative approaches based on experimental tests
- What competency has changed the most In the last 50 years?

Computing power has grown since 1970 by a factor of 10,000,000,000



The next decade according to Poursartip

- After more than 40 years of promise, the next decade will see an explosion in the use of composite materials as the major aerospace players, namely Boeing, Airbus and general aviation, have finally fully committed to this technology:
  - **The point of no-return has been crossed for aerospace**
- This commitment means that composites design and manufacturing technology will change dramatically, first in aerospace and then in all sectors as the technology permeates throughout the industry
  - **Automotive and alternative energy markets will follow**
- In ten years, no manufacturing company or material supplier will be untouched:
  - if in composites, they must stay competitive
  - if not in composites, they must ask whether another company can make their product in composites

Winds of change: Automotive

PURDUE ENGINEERING

BMW's Klaus Draeger says the i3 and larger i8 (pictured) will change the car making game forever

Juxtaposition of the Boeing 787 and carbon fiber automotive prototype

Why has it taken so long?

- New materials and processes present significant risks
- Uncertainty is at the heart of the matter
  - The number of possible combinations of polymers, constituents, interface designs and microstructures is huge
  - Edisonian approach to optimization
  - Product and material design is simultaneous
  - Ultra-conservative designs have been pervasive
  - Building block certification approach is very expensive
  - Certification is testing based ($millions/material)
  - Manufacturing is empirical, not science-based
  - Large scale integration of subassemblies to monocoque structures (too large to fail!)
  - Repair and joining technologies not robust

Variability and simulation

- Variability in composites comes from many sources
- Manufacturing and processing are among the dominant causes
- Simulation can capture variability
- Micromechanics and molecular mechanics can provide the links to variability
- Variability can be predicted

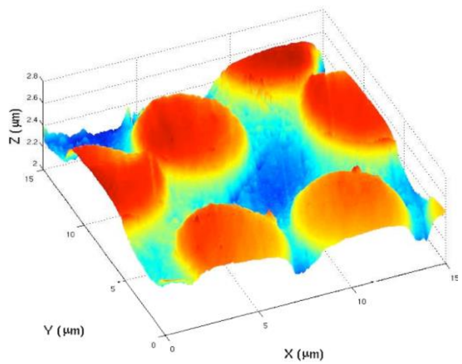
Simulation-based manufacturing

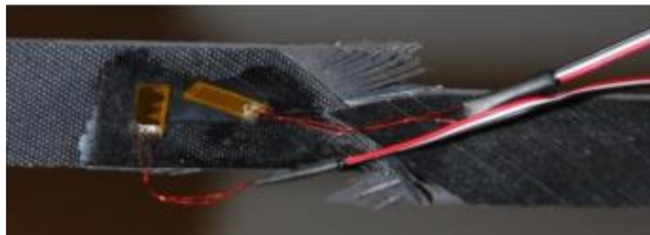
- The foundation tools for composites manufacturing simulation are available, but do not meet the broad range of needs
- The process for developing new manufacturing simulation tools are challenging.
- Accelerated development of design and simulation tools will require new approaches
- The economic incentive to accelerate composites manufacturing technology to a level consistent with mature industries such as automotive will continue unabated.

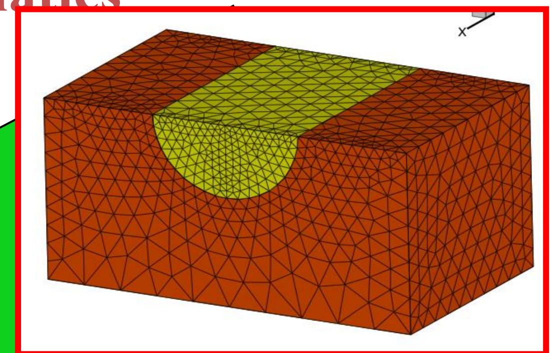
Multi-scale modeling approach

Characterization & Informatics

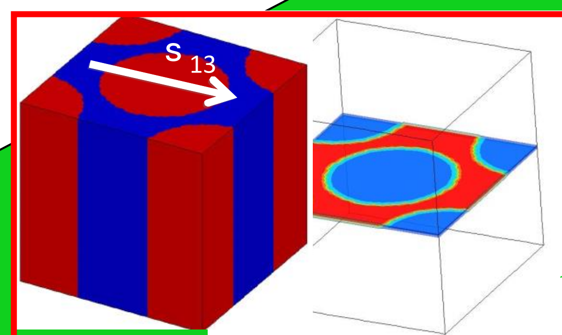
Nanometrology







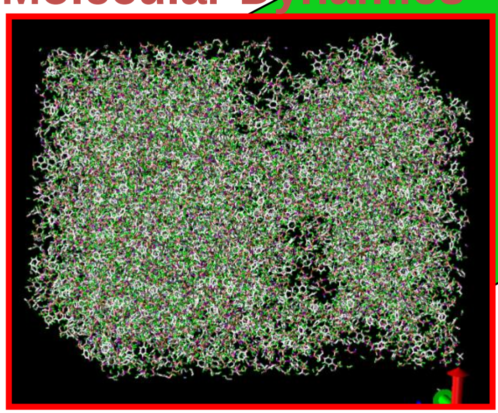
Finite Elements



Viscoelastic models

Phase field micromechanics

Molecular Dynamics

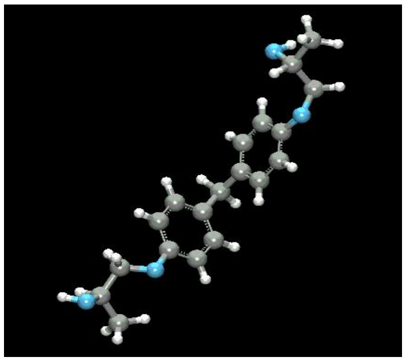


Viscoelastic models

<u>**Vision**</u>: predictive, validated models for design and certification of new materials

Molecular models of cross-linking polymers can connect synthesis to processing to properties

EPON 862



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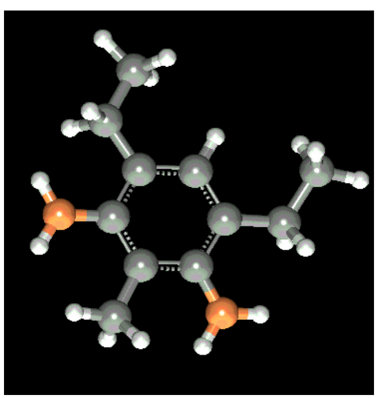
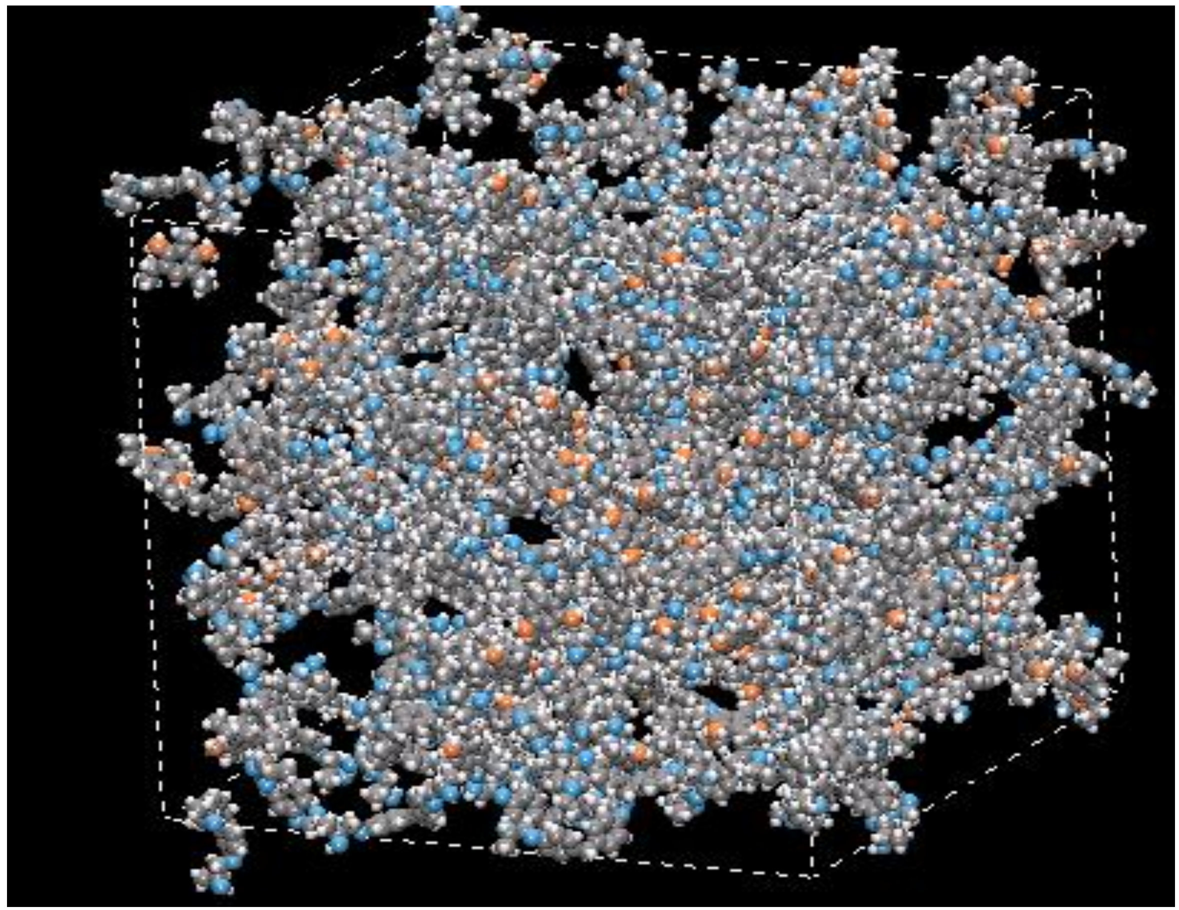
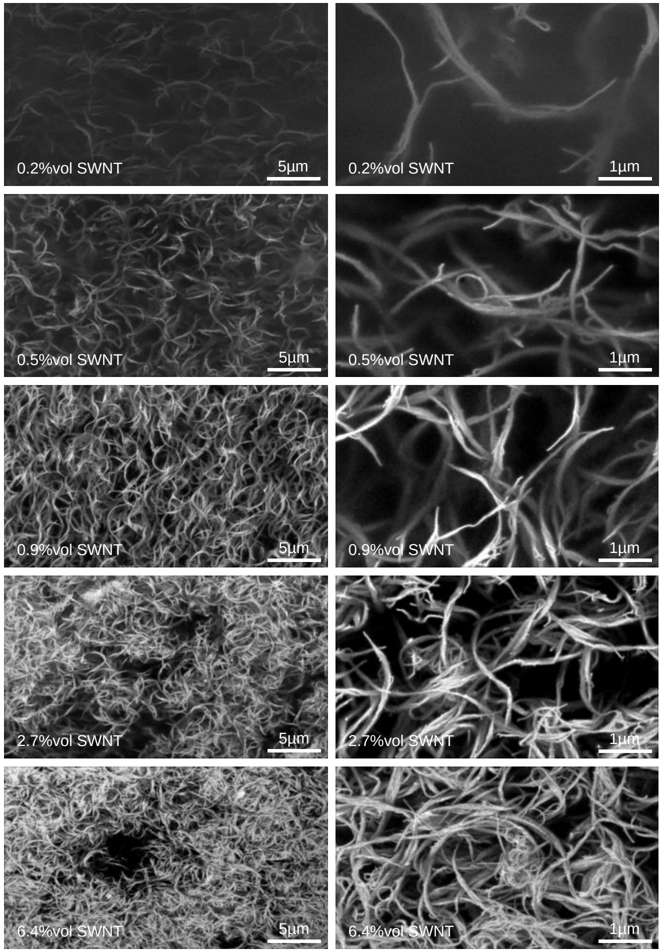




Multifunctional nanocomposites

- Simulation for optimum dispersion
- Accomplishing optimum dispersion remains the key challenge
-   Volume fraction at electrical percolation
-   Physical properties
-   Material forms
-   Interface



The Future is Polymer Composites!

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